

UNCLASSIFIED
AECU - 647

UNITED STATES ATOMIC ENERGY COMMISSION

SOME CALCULATED PROPERTIES OF TRITIUM

by
E. F. Hammel

Los Alamos Scientific Laboratory

Approved for Release: December 7, 1949

Contract No. W-7405-eng 36

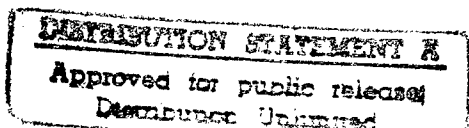
This document is reproduced as a project report
and is without editorial preparation. The manu-
script has been submitted to The Journal of Chem-
ical Physics for possible reproduction.

Styled, typed, and reproduced from copy
as submitted to this office.

Technical Information Division, ORE, Oak Ridge, Tennessee
AEC, Oak Ridge, Tenn., 2-24-50--675-A20959

PRINTED IN USA
PRICE 10 CENTS

UNCLASSIFIED



DTIC QUALITY INSPECTED 1

71-14501
NAVY RESEARCH SECTION
SCIENCE DIVISION
REFERENCE DEPARTMENT
LIBRARY OF CONGRESS

MAR 15 1950

SOME CALCULATED PROPERTIES OF TRITIUM

By S. F. Hammel

Application of quantum theory to the condensed permanent gases by J. De Boer¹ resulted in a modified law of corresponding states in terms of reduced P, V, and T variables, plus a parameter Λ^* . On the basis of this theory, De Boer and Lunbeck² predicted a number of properties of the helium isotope of mass three. Several of these properties, including the vapor pressure, were subsequently determined,³ and the experimental results agree quite closely with those predicted by De Boer and Lunbeck.² In the present paper, De Boer's theory is applied to tritium. Since the prediction of the He^3 properties involved a graphical extrapolation, whereas the prediction of the tritium properties involves an interpolation, it is hoped that an even closer agreement between theoretical and experimental results will be observed when data on tritium become available.

In Table 1, the constants pertinent to the calculation are collected. Corresponding values for H_2 and D_2 are included for comparison.

Table 1

| | Λ^* | ϵ/k (°K) | H/σ^3 (cm ³ /mol) | ϵ/σ^3 (atm) | ϵ (10 ⁻¹⁶ ergs) | σ (AU) |
|--------------|-------------|----------------------|--|------------------------------|--|------------------|
| H_2 | 1.73 | 37.0 | 15.12 | 203 | 50.75 | 2.92 |
| D_2 | 1.22 | 37.0 | 15.12 | 203 | 50.75 | 2.92 |
| T_2 | 1.00 | 37.0 | 15.12 | 203 | 50.75 | 2.92 |

Where $\Lambda^* = \frac{h}{\sigma \sqrt{m \epsilon}}$, k is Boltzmann's constant, H is Avogadro's number and σ and ϵ are characteristic quantities of the intermolecular field defined by the potential function representing the interaction between two molecules of the gas, viz:

$$\phi(r) = \epsilon \left\{ \frac{4}{(r/\sigma)^{12}} - \frac{4}{(r/\sigma)^6} \right\}$$

Thus for $r = \sigma$, $\phi(r) = 0$; and $\epsilon = \phi(r)$ for the value of r satisfying the equation $\partial\phi/\partial r = 0$. The variables of the reduced equation of state are defined in terms of "molecular" units as follows:

$$P^* = \frac{P\sigma^3}{\epsilon}, \quad V^* = V/N\sigma^3, \quad T^* = \frac{kT}{\epsilon}$$

The vapor pressures of tritium may be obtained from the theory by plotting experimental $\log P^*$ vs $1/T^*$ curves for the light elements as in Fig. 1; from this, a series of reduced isobars is constructed, viz., Fig. 2. From the latter graph, the vapor pressure vs temperature curve (Fig. 1 or Fig. 3) for tritium is immediately obtainable. The results are tabulated in Table 2 which also includes calculated data for deuterium above the boiling point.

Table 2*

| Tritium | |
|---------|-----------|
| T (°K) | P (mm Hg) |
| 12.2 | 0.154 |
| 13.3 | 0.488 |
| 14.3 | 1.54 |
| 15.6 | 4.88 |
| 17.1 | 15.4 |
| 18.9 | 48.8 |
| 20.2 | 95.1 |
| 21.3 | 154.4 |
| 21.58 | 181.2 |
| 22.2 | 233.8 |
| 23.0 | 322.6 |
| 24.2 | 488.0 |
| 25.0 | 643.5 |
| 26.0 | 867.3 |
| 27.0 | 1162.0 |
| 27.9 | 1544.0 |
| 33.9 | 4880.0 |

| Deuterium | |
|-----------------------|-----------|
| (Above boiling point) | |
| T (°K) | P (mm Hg) |
| 24.2 | 919.5 |
| 24.5 | 1007.5 |
| 25.0 | 1143.0 |
| 25.5 | 1304.0 |
| 26.0 | 1462.0 |

*Estimated uncertainty in the various temperatures associated with each vapor pressure: $\pm 0.3^\circ\text{K}$.

Using the modified law of corresponding states, a plot of a given reduced property vs Λ^* permits a prediction of that property for other substances with different Λ^* 's. In Table 3, the critical constants, triple-point constants, and several molecular constants for D_2 and T_2 so calculated are presented for comparison with corresponding experimental data for H_2 .

Table 3
Critical constants

| | T_c ($^{\circ}\text{K}$) | V_c (cm^3/mol) | P_c (atm) | | |
|--------------|------------------------------|------------------------------------|-------------|--|--|
| H_2 | 33.19† | 66.95† | 12.98† | | |
| D_2 | 41.1* | 56.7* | 18.9* | | |
| T_2 | 43.7* | 53.7* | 20.8* | | |

| Triple-point constants | | | | | |
|------------------------|------------------------------------|--|---|-------------------|---------------------|
| | T_{tr} ($^{\circ}\text{K}$) | V_{tr} (liquid)(cm^3/mol) | V_{tr} (solid)(cm^3/mol) | P_{tr} (atm) | P_{tr} (mm Hg) |
| H_2 | 13.96† | 26.10† | 23.25† | 0.071† | 53.7† |
| D_2 | 18.72† | 23.14† | 20.48† | 0.168† | 128.0† |
| T_2 | 21.65* | 21.90* | 19.24* | 0.248* | 188.0* |

| Molecular constants | | | |
|---------------------|------------------------------------|---------------------------------------|--------------------|
| | θ ($^{\circ}\text{K}$) | V_o (cm^3/mol) | U_o (cal/mol) |
| H_2 | 105* | 22.57* | 183† |
| D_2 | 97* | 19.49* | 276† |
| T_2 | 87† | 18.6† | 316† |

†Scott, Brickwedde, Urey, and Wahi, J. Chem. Phys. 2: 454 (1934).

‡Calculated by Dr. Boer's Theory.¹

From "Compilation of Thermal Properties of Hydrogen in its Various Isotopic and Other para Modifications," Woolley, Scott, and Brickwedde, J. Res. WBS 41: 379 (1948).

The value of U_o can be inserted into the theoretical equation for the vapor pressure, viz:

$$\log_{10} P = \frac{U_o}{2.303 RT} + 5/2 \log_{10} T + \text{Const.}$$

where the contribution of the thermal motion is neglected. This equation should be fairly accurate over a limited temperature range, especially at low temperatures. By choosing the constant equal to 2.130, an analytical representation of the calculated vapor pressures of solid tritium previously presented in Table 2 is obtained.

REFERENCES

1. Physica XIV: 139 (1948).
2. Physica XIV: 1101 (1948).
3. Syderiak, Grilly, and Hammel, Phys. Rev. 75: 303 (1949).

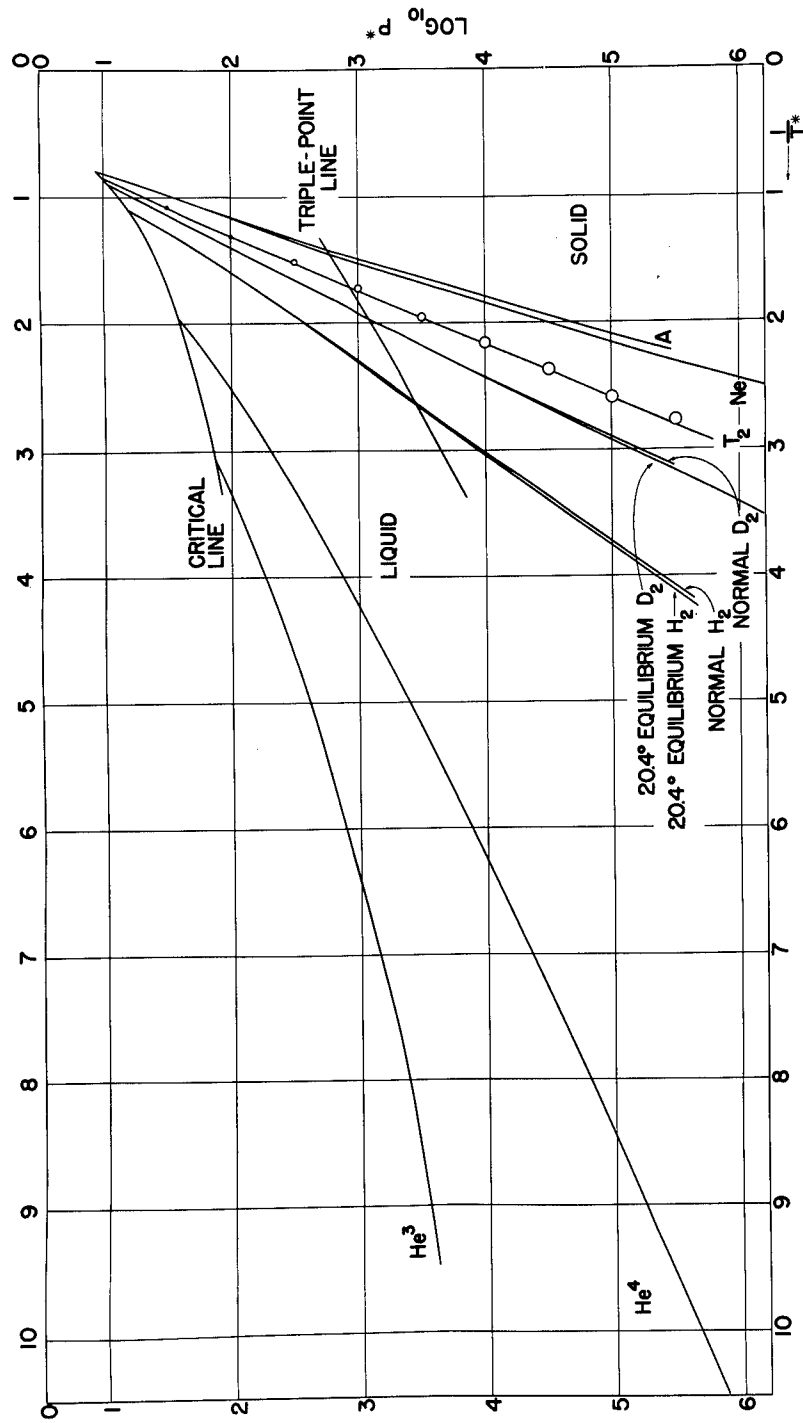
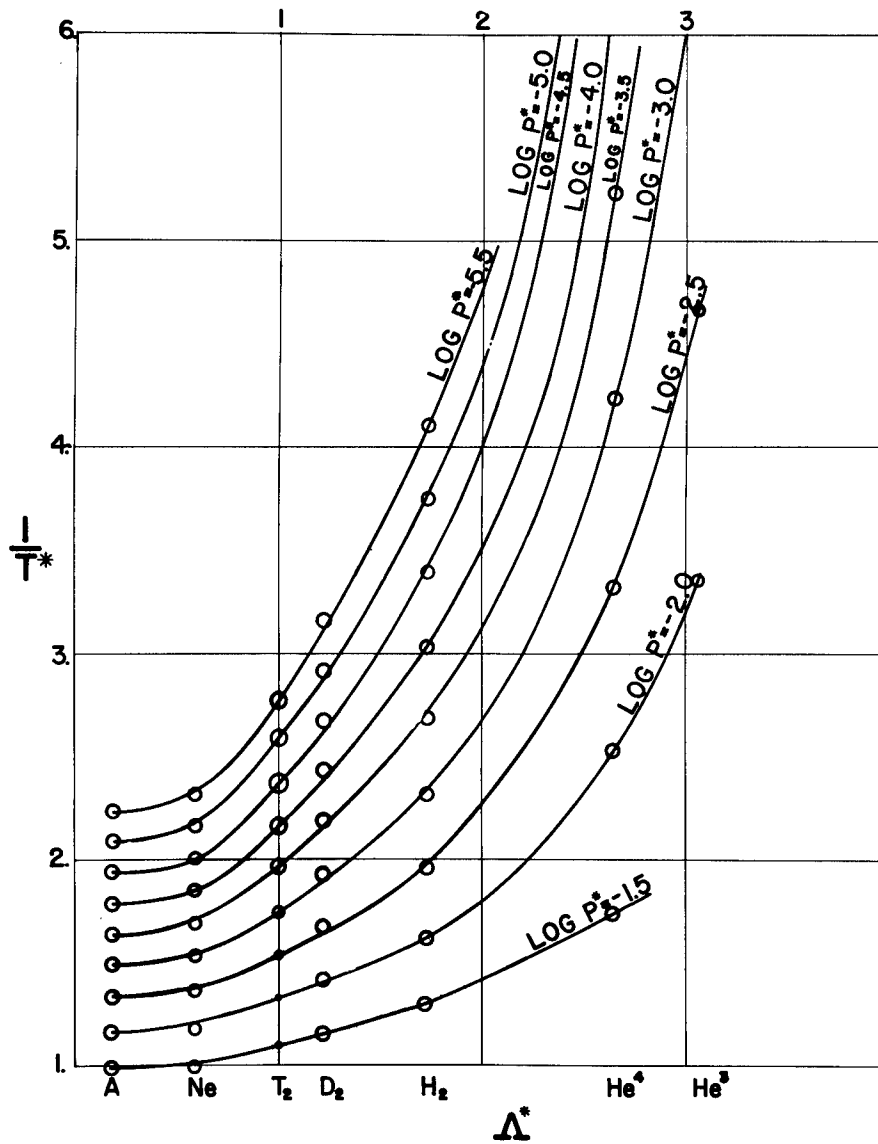


Fig. 1 — $\log_{10} P^*$ vs $1/T^*$ for various substances.

Fig. 2—Reduced isobars I/T^* vs Δ^* .

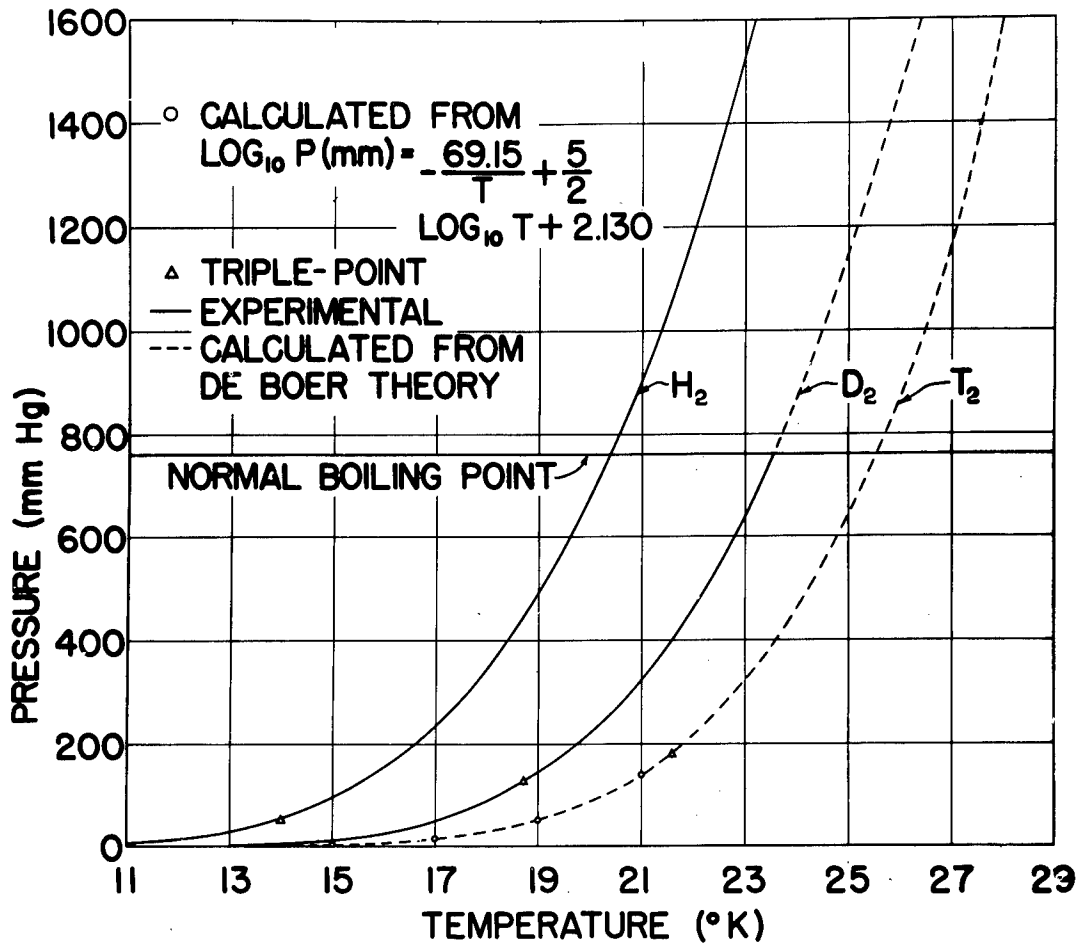


Fig. 3— Vapor-pressure curves of the hydrogen isotopes.

END OF DOCUMENT